

What is a Spectrum?

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Abstract. This contribution describes the “spectro-perfectionism” algorithm of Bolton & Schlegel (2010) that is being implemented within the Baryon Oscillation Spectroscopic Survey (BOSS) of the Sloan Digital Sky Survey III (SDSS-III), in terms of its potential to deliver Poisson-limited sky subtraction and lossless compression of the input spectrum likelihood functional given raw CCD data.

The Baryon Oscillation Spectroscopic Survey (BOSS) of the Sloan Digital Sky Survey III (SDSS-III Eisenstein et al. 2011) is the largest extragalactic spectroscopic survey to date, both in the number of spectra being collected and in the volume of the universe being mapped. BOSS has been delivering survey-quality spectra since December 2009, and is on track to obtain spectra of more than 1.5 million galaxies by mid-2014. While BOSS target galaxies are fainter than the galaxies observed in the original SDSS, the night-sky foreground is as bright as ever. This decreasing signal-to-foreground trend—which will only be exacerbated in future redshift surveys such as the proposed BigBOSS experiment (Schlegel et al. 2011)—demands a new approach to spectroscopic data analysis. This contribution to the proceedings describes the “spectro-perfectionism” algorithm of (Bolton & Schlegel 2010, hereafter B&S) in terms of its potential to deliver two important criteria for faint-object spectroscopy: (1) Poisson-limited night-sky foreground subtraction, and (2) lossless likelihood functional compression. The B&S algorithm is based upon extraction via forward-modeling to the raw CCD data using the full two-dimensional (2D) point-spread function (PSF) of the spectrograph, and is currently in the software implementation phase for eventual deployment within the BOSS survey.

The current state of the art for extraction of spectra in optical astronomy is the *optimal extraction* method described by Hewett et al. (1985) and Horne (1986), which models the spectrum in each successive CCD pixel row (corresponding to a particular effective wavelength) via a maximum-likelihood scaling of a spatial cross-sectional profile. The shortcomings of this method can best be understood by considering how it extracts an emission line, such as one of the OH features that are prominent redward of 7000 Å. If the PSF is a non-separable function of x and y in CCD coordinates (such as will be the case for a PSF consisting of a core plus wings, or a PSF with significant tilted ellipticity and/or skewness), then the actual spatial cross-sectional profile will depend upon the location of the cross section within the spectrum (e.g., a cross section through the wing will be broader than a cross section through the core). By extracting with a single mean profile $p(x)$ rather than the true cross-sectional profile $q(x)$ in a given row,

a fractional bias in the extracted counts is introduced which is given by

$$b = 1 - \left[\int dx p(x)q(x) \right] \left[\int dx q^2(x) \right]^{-1}. \quad (1)$$

In practice this bias may be small, but when coupled to variations in the spectrograph PSF across the field of view of a multifiber spectrograph, it can result in significant systematic residuals after the subtraction of a model sky spectrum. For very faint galaxy spectroscopy, we wish to push these residuals well below the 1% level, and hence we are pursuing extraction using the mathematically correct forward model given by the 2D PSF rather than the mean 1D cross-section. Given a sufficiently accurate model for the PSF and its variation across the instrument, we can construct a noise-limited model for the raw CCD data, and can furthermore model the common sky spectrum *upstream* from the variation of the PSF.

To realize the full benefit of 2D PSF-based extraction, we develop a mathematically explicit answer to the question: what is a spectrum? Let the vector \mathbf{f} represent an extracted 1D spectrum in the sense commonly understood in astronomy. Its most important function is to permit quantitative inference about the object under observation. For this purpose, the full information content of the spectrum is not only in the vector \mathbf{f} , but also in the estimate of its noise properties and its resolution. We will represent the noise by the statistical covariance matrix \mathbf{C} of the pixels in the spectrum, and the resolution by a matrix \mathbf{R} that encodes the “line-spread function” (LSF) of the spectrum. If it is diagonal, \mathbf{C} can be represented by a vector of pixel errors (and this is often assumed even when it is not true). The matrix \mathbf{R} represents the instrumental “blurring” of an input spectrum, and is ideally band diagonal, with a bandwidth that is neither too large (oversampled) nor too small (undersampled). All the inferential power of the spectrum is encapsulated by the “likelihood functional” of a model spectrum \mathbf{m} given the data, which if we assume Gaussian noise can be expressed by the χ^2 statistic:

$$\chi_{\text{spec}}^2(\mathbf{m} \mid \text{data}) = (\mathbf{f} - \mathbf{R}\mathbf{m})^T \mathbf{C}^{-1} (\mathbf{f} - \mathbf{R}\mathbf{m}). \quad (2)$$

Let us now consider the raw data and calibrations from which \mathbf{f} , \mathbf{C} , and \mathbf{R} are derived. Generally speaking, the predicted counts c_i in CCD pixel i (where i is a single index that is understood to run over rows, columns, and multiple CCDs) may be related to the input model spectrum $m(\lambda)$ through the linear relation

$$c_i = \int d\lambda A_i(\lambda) m(\lambda), \quad (3)$$

where $A_i(\lambda)$ is a transfer function for pixel i . If we assume sufficient finite sampling points of the spectrum and transfer function in the wavelength domain indexed by j , we may represent the operation of the telescope, instrument, and detector by a matrix relationship

$$c_i = A_{ij} m_j. \quad (4)$$

Here, the matrix \mathbf{A} , which we shall refer to as the “calibration matrix”, generalizes and incorporates the spectrum trace solution, wavelength solution, 2D spectrograph PSF, relative and absolute throughput variation, variations in CCD pixel sensitivity, and all other calibration considerations that are generally considered separately from one another. The problem of accurately estimating \mathbf{A} given standard calibrations (i.e., arcs

and flats, as well as science frames for self-calibration) is perhaps the most challenging aspect of spectroscopic data reduction. The strategy for determining \mathbf{A} is beyond the scope of this contribution; here we only note that in most instrumental contexts, the calibration matrix will have sufficient symmetry, sparsity, and smoothness to make its estimation a well-constrained problem (Pandey 2011).

If we assume that \mathbf{A} has been determined, that we have a set of measured science CCD pixel counts represented by the vector \mathbf{p} , and that the associated (uncorrelated) squared pixel errors constitute the diagonal raw-pixel covariance matrix \mathbf{N} , the likelihood functional of any model input spectrum vector \mathbf{m} is represented by

$$\chi_{\text{raw}}^2(\mathbf{m} \mid \text{data}) = (\mathbf{p} - \mathbf{A}\mathbf{m})^T \mathbf{N}^{-1} (\mathbf{p} - \mathbf{A}\mathbf{m}), \quad (5)$$

and in principle any and all inference can be made directly against the raw pixels. In practice this approach is generally both onerous and unnecessary. However, the obvious analogy between Equations 2 and 5 suggests the following operational definitions for three commonly understood stages of spectral data analysis:

Calibration	\equiv	Likelihood functional determination
Extraction	\equiv	Likelihood functional compression
Measurement	\equiv	Likelihood functional projection

The quality of an extraction algorithm can thus be judged by the lossiness of its compression of the input-spectrum likelihood functional through the translation of χ_{raw}^2 (as specified by \mathbf{A} , \mathbf{N} , and \mathbf{p}) into χ_{spec}^2 (as specified by \mathbf{R} , \mathbf{C} , and \mathbf{f}).

To arrive at a lossless extraction algorithm, note first that we can approach Equation 5 naively to determine a maximum-likelihood (minimum- χ^2) solution for the *input* spectrum \mathbf{m} as

$$\mathbf{m}_{\text{m.l.}} = (\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A})^{-1} (\mathbf{A}^T \mathbf{N}^{-1}) \mathbf{p}. \quad (6)$$

However, this estimator has undesirable properties as an extracted spectrum. The square matrix $(\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A})^{-1}$, being the inverse of the symmetric banded non-negative matrix $\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A}$, will have significant bandwidth and large positive/negative fluctuations off the diagonal. Since this is the covariance matrix of the sample elements of $\mathbf{m}_{\text{m.l.}}$, the estimated spectrum will exhibit significant ringing. This is an expected consequence of the deconvolution implicit in the solution for $\mathbf{m}_{\text{m.l.}}$.

This deconvolution problem highlights an apparent advantage of the row-by-row optimal extraction algorithm: while row-by-row deconvolves the 2D spectrum image in the spatial direction (on the strong prior assumption that the input signal is a one-dimensional spectrum distributed according to a known profile), it does not deconvolve the instrumental profile in the wavelength direction, and hence introduces no ringing. The price, as seen above, is that this computation is carried out using a mathematically incorrect model for the projection of photons onto the detector. One solution in the context of 2D PSF extraction would be to impose a regularizing prior on $\mathbf{m}_{\text{m.l.}}$. However, regularization of the input spectrum model is the purview of science analysis, not of data reduction. If implemented at this stage, it would break the model of extraction as likelihood functional compression.

To proceed, consider a diagonalization of the matrix $\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A}$ as

$$\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A} = \mathbf{R}^T \mathbf{C}^{-1} \mathbf{R}, \quad (7)$$

where \mathbf{R} is a square matrix (in contrast to \mathbf{A} , which has many more rows than columns) and \mathbf{C}^{-1} is a diagonal matrix. This diagonalization need not necessarily be in the eigen-decomposition sense. To factorize in the sense described in B&S, we first consider the matrix \mathbf{U} whose columns are the eigenvectors of $\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A}$, and the corresponding diagonal matrix \mathbf{E} of eigenvalues. Since the original matrix is real, symmetric, and positive definite, \mathbf{U} is orthogonal, with its inverse equal to its transpose, and all its eigenvalues are real and positive. Now we define

$$\mathbf{R} \equiv \mathbf{S} \mathbf{U} \mathbf{E}^{1/2} \mathbf{U}^T \quad (8)$$

$$\mathbf{C} \equiv \mathbf{S}^2, \quad (9)$$

where $\mathbf{E}^{1/2}$ is a diagonal matrix whose entries are the positive square roots of the entries of \mathbf{E} , and \mathbf{S} is a diagonal matrix defined so that \mathbf{R} is normalized to unity in each row when summed over columns. (The more intuitive “flux-conserving” normalization associated with a sum over rows is less straightforward to implement.) With this definition of \mathbf{R} and \mathbf{C} , Equation 7 is satisfied exactly. We have diagonalized the (inverse) covariance matrix, opting not for the orthogonality of \mathbf{U} , but rather for the band-diagonal locality of \mathbf{R} , which derives from its relationship to the matrix square root of the band diagonal matrix $\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A}$. That is to say, the matrix \mathbf{R} by our definition will “look like” a line-spread function in the sense understood in astronomical spectroscopy.

We note in passing that the definition of \mathbf{R} that we have adopted, while well motivated, is not unique. In fact, the motivation for a smoothly varying line spread function with wavelength may even be worth accepting a small degree of off-diagonal covariance. A desire for a flux-conserving definition of \mathbf{R} may also motivate different choices. As noted by B&S, cross-talk between neighboring spectra of a multiobject spectrograph presents additional complication. The particular choices and approximations adopted will necessarily be driven by instrumental and scientific context.

Finally, we define our extracted spectrum \mathbf{f} as the “reconvolution” of our deconvolved extraction by the resolution matrix \mathbf{R} , thereby removing the ringing:

$$\mathbf{f} \equiv \mathbf{R} \mathbf{m}_{\text{m.l.}} = \mathbf{R} (\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A})^{-1} (\mathbf{A}^T \mathbf{N}^{-1}) \mathbf{p}. \quad (10)$$

Now, using the definitions of \mathbf{R} , \mathbf{C} , and \mathbf{f} given in Equations 8–10, we find that χ_{spec}^2 as given by Equation 2 is equal up to a constant offset to χ_{raw}^2 as given by Equation 5 *for any trial model spectrum* \mathbf{m} . Thus we attain the goal of extraction as lossless likelihood-functional compression, with \mathbf{A} , \mathbf{N} , and \mathbf{p} replaced respectively by the band-diagonal LSF matrix \mathbf{R} , the diagonal spectrum covariance matrix \mathbf{C} (i.e., an error vector), and the flux vector \mathbf{f} . Equally important is the fact that \mathbf{R} , \mathbf{C} , and \mathbf{f} collectively satisfy the intuitive understanding of “a spectrum” in the astronomer’s sense!

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